Comment on fractality of quantum mechanical energy spectra

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The fractal properties of the energy spectra of quantum systems are discussed in connection with the paper by Sáiz and Martínez [Phys. Rev. E **54**, 2431 (1996)]. It is shown that for discrete energy levels the Hausdorff–Besicovitch dimension is zero and differs from the Renyi scaling exponents computed by the standard box counting algorithm. The Renyi exponents for the inverse power series data sets ($x_n = \frac{1}{n^a},\ n = 1, 2, \ldots$) are computed analytically and they are shown to be $d_0 = \frac{1}{1+a}$ and, as a consequence, $d_0 = 1/3$ for the Balmer formula.

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In last years there is an increasing interest in searching for fractal structures in physics [1] and in looking for fractal signatures of chaos at the quantum mechanical (QM) level [2,3,4], as well. In fact, a simple QM system with fractal energy spectrum has been found long time ago [5]. Similar structures have been found in recent years in other systems that are of great practical importance: the quasiperiodic semiconductor microstructures, the quantum Hall effect and the Anderson localization [6,7]. In this paper I would like to comment on possible fractality of QM spectra and I will discuss Renyi exponents [8,9] for some special types of point spectra generated by simple probability distributions, as well as for Balmer like energy levels computed in [3]

$$E_n \sim \left(\frac{1}{m^2} - \frac{1}{n^2}\right) \ , \quad n > m \ , \quad m = 1, 2, 3, 4, 5 \ . \quad (1)$$

Typical QM systems have either discrete point spectra (localized states, like for the harmonic oscillator), continuous spectra (extended states, like for the free particle) or both (localized and extended states above some threshold energy, like for the hydrogen atom). In addition, the models have been found that have neither extended nor localized states and their energy spectra have been shown to be fractal [5,6,7]. These are models that describe infinite crystals (periodic or almost periodic). In this paper I will limit discussion to the case of discrete spectra.

For the discrete spectra it has been shown that their nearest neighbor spacing (NNS) of energy levels has Poisson or Wigner probability distribution (for corresponding chaotic Hamiltonians) [10,11]. Such spectra cannot lead to any fractal structure as any reasonable probability distribution cannot give the Cantor like structures (in particular, the Poisson, Wigner or Thomas–Porter distributions are regular enough). On the other hand, the energy spectra with finite number of accumulation points cannot be generated by a reasonable (regular) probability distribution. However, using the correct definition of the fractal (Hausdorff–Besicovitch) dimension [12,13] one can easily show that for any set with finite number of accumulation points the Hausdorff–Besicovitch dimension is zero, $d_H = 0$. Hence, for any nuclear or molecular discrete energy spectra we should get their fractal dimension equal to zero.

In practical (numerical) calculations of the fractal dimension the box counting algorithm and the Renyi exponents (improperly called "dimensions") are used [14]. The whole interval is divided into N equal subintervals ("boxes") with $n_i(N)$ ($i = 1, 2, \ldots, N$) data points in each box. Defining the measure $p_i(N) = n_i(N)/n_{tot}$, where $n_{tot} = \sum_i n_i(N)$ is the total number of data points, we have the following definition of the Renyi exponents

$$d_q = \frac{-1}{q-1} \lim_{N\to\infty} \frac{\ln \sum_i p_i^q(N)}{\ln N} \ . \quad (2)$$

Here, for $q = 0$ (the capacity "dimension") we assume summation over non–empty boxes only, and (2) becomes equivalent to

$$d_0 = \lim_{N\to\infty} \frac{\ln M(N)}{\ln N} \ , \quad (3)$$

where $M(N)$ is the total number of non–empty boxes. For $q = 1$ (the information "dimension") the de l'Hospital rule is applied to the formula (2) and one gets

$$d_1 = -\lim_{N\to\infty} \frac{\sum_i p_i(N) \ln p_i(N)}{\ln N} \ . \quad (4)$$

Once again, it is important to remember that the Renyi exponents are *not* the (fractal) dimensions and for some "pathological" sets they may differ from the Hausdorff–Besicovitch dimension [12,13]. In particular, this happens for the inverse power like discrete sets, as will be shown below. However, even for such pathological sets one can use the Renyi exponents just to describe the scaling properties of the data. With this remark in mind we

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prove the following
Theorem: For the inverse power series $x_n = 1/n^a$, where $n = 1, 2, 3, \ldots$ and $a > 0$ the Renyi exponent d_0 is

$$d_0 = \frac{1}{1+a} \ . \tag{5}$$

Proof: Let us denote by n_{sngl} the number of points that are single in their boxes. We have $M(N) \geq n_{sngl}$ and, from the condition $x_n - x_{n+1} \geq 1/N$ (distance between such points is greater than the box size $= 1/N$), we get $n_{sngl} = a^{\frac{1}{1+a}} N^{\frac{1}{1+a}}$. In fact, in the last equation there should be taken integer part of the right hand side but this is unimportant as we are interested in the limit $N \to \infty$. Using the definition 2 with $q = 0$ one gets asymptotically for $N \to \infty$ the lower limit $d_0 \geq (a+1)^{-1}$. To get the lower limit we took into account points in the interval $[x_{sngl}, 1]$, $x_{sngl} = x_{n_{sngl}} = 1/n^a_{sngl}$. To obtain an upper limit we have to take into account the remaining boxes as well. First, let us notice that the first box, *i.e.* the interval $[0, 1/N]$ contains infinite number of points for any N, as zero is the accumulation point, and the interval $[1/N, x_{sngl}]$ contains at most $(x_{sngl} - 1/N)/(1/N)$ non–empty boxes. This gives the following upper limit for $M(N)$

$$M(N) \leq a^{\frac{1}{1+a}} \left(1 + \frac{1}{a}\right) N^{\frac{1}{1+a}} \ ,$$

and, as a consequence, we have

$$d_0 \ \leq \ \lim_{N\to\infty} \frac{\ln\left[a^{\frac{1}{a+1}} \left(1+\frac{1}{a}\right) N^{\frac{1}{a+1}}\right]}{\ln N} \ = \ \frac{1}{a+1} \ .$$

Hence, we have proven the eq. (5).

This result gives us the scaling exponent $d_0 = 1/2$ for the harmonic series (as was stated in [3]), while for the Balmer like series ($a = 2$) we have $d_0 = 1/3 \simeq 0.33$, in contrast to the result presented in [3], where the value 0.61 was obtained numerically. Of course, neither the Hausdorff–Besicovitch dimension nor the Reny exponent be can changed by the overall shift of the whole set (due to the $1/m^2$ term in (1)), or by rejection of any finite number of the data points ($n > m$), or even by superposition of any finite number of such sets (as we have in (3) logarithm in the numerator). In fact, superposition of two fractal sets has the fractal dimension equal to the maximum fractal dimension of the constituent sets [13]. Hence, our result cannot be changed by any simple composition of Balmer like sets.

I have done some numerical checks of the analytical result (5) with the box counting algorithm and both methods are consistent. In particular, for $a = 2$ and 1000 data points the box counting method gives: $d_0 \simeq 0.321$, where 6 points fit to the straight line with $\chi^2 \simeq 0.0072$ and the correlation parameter $r \simeq 0.99988$ (the finest division was $N = 2^{25}$).

Finally, I would like to mention that the modified scaling exponents were suggested to investigate QM systems with discrete spectra [2,4]. Namely, the probabilities $p_i(N)$ obtained by the simple level–counting in a box have been changed by summation of the de–excitation probabilities. In this case, not only the information contained in the energy spectrum but also in eigenfunctions is employed. However, even in this case, up to now, we are unable to find any interesting physical interpretation of the scaling exponents.

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